

# On the use of stochastic differential geometry for non-equilibrium thermodynamics modeling and control

Paolo Muratore-Ginanneschi

*Department of Mathematics and Statistics, University of Helsinki PL 68, 00014 Helsinki, Finland.*

We discuss the relevance of geometric concepts in the theory of stochastic differential equations for applications to the theory of non-equilibrium thermodynamics of small systems. In particular, we show how the Eells-Elworthy-Malliavin covariant construction of the Wiener process on a Riemann manifold provides a physically transparent formulation of optimal control problems of finite-time thermodynamic transitions. Based on this formulation, we turn to an evaluative discussion of recent results on optimal thermodynamic control and their interpretation.

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## INTRODUCTION

Stochastic differential equations [19] provide a widely applied mathematical model for non-equilibrium dynamics. In particular, they are well adapted to the description of kinetics and finite time thermodynamics of small systems such as bio-molecules, RNA and other molecular scale “machines”, see e.g. [38] for review of theoretical and experimental aspects. The application of stochastic differential equations to non-equilibrium phenomena bears a natural relation to geometry in an, at least, twofold way. First, even when a stochastic differential equation is used to model processes evolving in a flat, Euclidean, space, in *arbitrary coordinates* the scale of the noise in the stochastic differential equation imposes a Riemannian or sub-Riemannian (if there are constraints on the admissible directions of motion such as conditioning a set of variables to be the derivatives of other ones) metric on the space. The second way geometry sets in is more distinctive of applications to non-equilibrium physics. It originates from the use of second derivatives of thermodynamic potentials to impose a Riemannian metric on the set of equilibrium states. The consequent notion of thermodynamic length has been then exploited to characterize optimal processes in macroscopic and, very recently, microscopic, nano-scale processes (see [43] for references and discussion). In the present contribution we show how a coordinate-independent geometric formalism may ease the analysis of control problems arising in the study of finite-time thermodynamics of small systems. Although the needed mathematical tools are well known in stochastic analysis (see e.g. [5, 16, 19, 37]), we are not aware of any previous application to stochastic thermodynamics. In what follows we will generically denote by  $\mathbb{M}$  a complete connected Riemannian manifold. We will also imply some further technical assumptions to guarantee probability conservation (see e.g. [17] for concise discussion). In practice, our main focus here will be on covariance of physical laws so that  $\mathbb{M}$  can be thought as  $\mathbb{R}^d$  endowed with a Riemannian metric. Finally, in order

to simplify the notation, thermodynamic expressions will be evaluated at unit temperature.

## GEOMETRY AND THE DEVELOPMENT MAP

Differential geometry is most naturally formulated in the language of first order forms. For this reason Stratonovich calculus [19] is commonly considered to have an edge on Ito calculus when it comes to identify geometric structures. Let us therefore start by considering a diffusion process  $\boldsymbol{\xi} \equiv \{\boldsymbol{\xi}_t; t \in [t_o, t_f]\}$  specified by stochastic differential equations in the sense of Stratonovich

$$d\boldsymbol{\xi}_t = \mathbf{b}_S(\boldsymbol{\xi}_t, t) dt + \mathbf{e}_i(\boldsymbol{\xi}_t) \diamond d\beta_{i;t} \quad (1)$$

in a coordinate neighborhood  $\mathbb{U} \in \mathbb{M}$  centered e.g. around the initial condition  $\boldsymbol{\xi}_{t_o} = \mathbf{x}_o$ . The symbol  $\diamond$  pinpoints the Stratonovich prescription. In (1)  $\mathbf{b}_S: \mathbb{U} \times [t_o, t_f] \mapsto \mathbb{R}^d$  is some smooth *map*, Einstein convention is implied on the latin indices  $i = 1, \dots, d$  to pair the elements of a collection of  $d$  independent one-dimensional Euclidean Wiener processes (Brownian motions)  $\beta_i \equiv \{\beta_{i;t}; t \in [t_o, t_f]\}$  to  $d$  orthonormal frame fields  $\{\mathbf{e}_i\}_{i=1}^d$  specifying a basis for  $T_{\boldsymbol{\xi}_t}\mathbb{M}$ . Let us also endow  $\mathbb{M}$  with a strictly positive, time-independent metric tensor  $\mathbf{g}$  and require that for any  $\mathbf{x} \in \mathbb{U}$

$$\langle \mathbf{e}_i, \mathbf{e}_j \rangle_{\mathbf{g}} := \mathbf{g}_{\alpha_1 \alpha_2} \mathbf{e}_i^{\alpha_1} \mathbf{e}_j^{\alpha_2} = \delta_{ij} \quad (2)$$

( $\alpha_j = 1, \dots, d, j = 1, 2$ ) which is equivalent to

$$\mathbf{e}_i \otimes \mathbf{e}_i = \mathbf{g}^{-1} \quad (3)$$

The hypothesis of time-independence of the metric tensor is physically relevant and will also serve later to neaten the formalism. The extension to the time dependent case is, however, straightforward and it is of common use for example in the inquiry of Ricci flows, see e.g. [8, 44] for details. From (1) we can write for any  $\mathbf{x} \in \mathbb{U}$  the

generator of the stochastic process  $\mathbf{x}$  acting on any *scalar function*  $f : \mathbb{U} \mapsto \mathbb{R}$

$$\begin{aligned} \mathfrak{L}_S f &= \left( \mathbf{b}_S \cdot \partial_{\mathbf{x}} + \frac{1}{2} \mathbf{e} \cdot \partial_{\mathbf{x}} \mathbf{e} \cdot \partial_{\mathbf{x}} \right) f = \\ &= \left\{ \left[ \mathbf{b}_S + \frac{1}{2} (\mathbf{e}_i \cdot \partial_{\mathbf{x}} \mathbf{e}_i) \right] \cdot \partial_{\mathbf{x}} + \frac{1}{2} \mathbf{g}^{-1} : \partial_{\mathbf{x}} \otimes \partial_{\mathbf{x}} \right\} f \end{aligned} \quad (4)$$

( $\mathbf{b} \cdot \partial_{\mathbf{x}} \equiv \mathbf{b}^{\alpha_1} \partial_{x^{\alpha_1}}$  and  $\mathbf{A} : \mathbf{B} \equiv \text{Tr} \mathbf{A}^\dagger \mathbf{B}$ ). The last equality in (4) motivates the identification of the inverse of the metric as the diffusion tensor of the process  $\boldsymbol{\xi}$ . A diffusion process is fully specified by the knowledge of the conditional expectation of its increments up to second order. Under the present hypotheses these expectation values are

$$\begin{aligned} \lim_{dt \downarrow 0} \mathbb{E}_{\mathbf{x}, t} \left\{ \frac{\boldsymbol{\xi}_{t+dt} - \boldsymbol{\xi}_t}{dt} \right\} &= \\ \left( \mathbf{b}_S + \frac{1}{2} (\mathbf{e}_i \cdot \partial_{\mathbf{x}} \mathbf{e}_i) \right) (\mathbf{x}, t) &:= \mathbf{b}_I(\mathbf{x}, t) \end{aligned} \quad (5)$$

the “Itô drift”, and

$$\lim_{dt \downarrow 0} \mathbb{E}_{\mathbf{x}, t} \left\{ \frac{(\boldsymbol{\xi}_{t+dt} - \boldsymbol{\xi}_t) \otimes (\boldsymbol{\xi}_{t+dt} - \boldsymbol{\xi}_t)}{dt} \right\} = \mathbf{g}^{-1}(\mathbf{x}) \quad (6)$$

the diffusion tensor. It is therefore physically justified to take (5) and (6) as the *data* specifying a stochastic differential equation. We are now in the position to pinpoint two disadvantages related to the use of (1). For any  $\mathbf{O} \in O(d)$ , the group of orthogonal matrices, the vector-valued Wiener processes  $\boldsymbol{\beta} := [\beta_1, \dots, \beta_d]$  and  $\mathbf{O}\boldsymbol{\beta}$  are statistically equivalent. Let us denote with  $O(\mathbb{M})$  the collection of  $d$ -tuples  $[\mathbf{x}, \mathbf{e}_1(\mathbf{x}), \dots, \mathbf{e}_d(\mathbf{x})]$  attached to any  $\mathbf{x} \in \mathbb{M}$ . In the language of differential geometry, this collection forms the “bundle” of orthonormal frames specified by the triple  $(O(\mathbb{M}), O(d), \mathbb{M})$  [18, 19]. Since only (6) is observable, any element of the bundle must provide an equivalent description of the statistics of the process  $\boldsymbol{\xi}$ . Equation (1), however, is not invariant for different choices of orthonormal frames in the bundle. More explicitly, the same statistics can be equivalently described by the Stratonovich drift  $\mathbf{b}_S$  or by its “gauge” transform

$$\mathbf{b}_S[\mathbf{O}] = \mathbf{b}_S - \frac{1}{2} (\mathbf{O}_{i_1 i_1} (\mathbf{e}_{i_1} \cdot \partial_{\mathbf{x}}) \mathbf{O}_{i_2 i_2}) \mathbf{e}_{i_2} \quad (7)$$

This fact was already noted long ago in connection to the inquiry of the covariant path-integral representation of stochastic processes and Euclidean Quantum Mechanics over curved manifolds (see e.g. [14, 20] and [33] for a more complete list of references). A second disadvantage is that the natural, coordinate independent, definition of the generator of  $\boldsymbol{\xi}$  acting on *scalar functions* is [21, 22]

$$\mathfrak{L} = \left( \mathbf{b} \cdot \partial_{\mathbf{x}} + \frac{1}{2} \Delta_{LB} \right) f \quad (8)$$

with  $\Delta_{LB}$  the Laplace-Beltrami operator and  $\mathbf{b}$  a vector field which we will refer to as the covariant drift. In general, it is not possible to identify globally on  $\mathbb{M}$  the Stratonovich drift with the covariant one i.e.  $\mathbf{b}_S = \mathbf{b}$  unless the integrability condition

$$\mathbf{v}_1 \cdot \partial_{\mathbf{x}} \langle \mathbf{v}_2, \mathbf{e} \rangle_{\mathbf{g}} = \mathbf{v}_2 \cdot \partial_{\mathbf{x}} \langle \mathbf{v}_1, \mathbf{e} \rangle_{\mathbf{g}} \quad (9)$$

is satisfied for any *constant* vectors  $\mathbf{v}_1, \mathbf{v}_2$ . To interpret (9) we observe that it is satisfied if there exists a collection of scalar functions  $\{G_i\}_{i=1}^d$  such that

$$\partial_{\mathbf{x}} G_i = \mathbf{g} \cdot \mathbf{e}_i \quad (10)$$

whence it follows that

$$\langle \mathbf{e}_i, d\boldsymbol{\xi}_t \rangle_{\mathbf{g}} = dG_i(\boldsymbol{\xi}_t) \quad (11)$$

meaning that there exists a change of variables turning in (4) the frame fields  $\{\mathbf{e}_i\}_{i=1}^d$  into the canonical basis of  $\mathbb{R}^d$ . In other words, (10) states the existence of a privileged choice of global coordinates for which the noise becomes additive. In general, however, (9) is not satisfied since

$$\Delta_{LB} f = \mathbf{g}^{-1} : \partial_{\mathbf{x}} \otimes \partial_{\mathbf{x}} f - (\Gamma : \mathbf{g}^{-1}) \cdot \partial_{\mathbf{x}} f \quad (12)$$

with  $\Gamma$  the Christoffel symbols of the Levi-Civita connection on  $\mathbb{M}$ . In [21] Itô gave the expression in local coordinates of a stochastic differential equation (in Itô sense) associated to (8)

$$d\boldsymbol{\xi}_t = \left( \mathbf{b} - \frac{1}{2} \Gamma : \mathbf{g}^{-1} \right) dt + \mathbf{e}_i d\beta_{i;t} \quad (13)$$

A straightforward calculation shows then that (1) is equivalent to (13) if (9) is satisfied. The conclusion is that the Stratonovich equation (1) does not provide a coordinate-independent description of the dynamics. Furthermore, inspection of (13) shows that the “Itô drift” cannot transform as vector field under general change of coordinates. The Eells-Elworthy-Malliavin development map (see e.g. [5, 16, 19] for rigorous *and* pedagogic derivations) obviates these disadvantages. The idea is that a Wiener process can be path-wise constructed on  $\mathbb{M}$  by “rolling” the manifold along the realizations of an Euclidean Brownian motion. Mathematically this means that the Wiener process should be constructed as the solution of the *system* of Stratonovich differential equations

$$d\boldsymbol{\omega}_t = \mathbf{e}_i \diamond d\beta_{i;t} \quad (14a)$$

$$d\mathbf{e}_{i;t} = -\Gamma : \mathbf{e}_{i;t} \overset{\diamond}{\otimes} d\boldsymbol{\omega}_t \quad (14b)$$

As above, the  $\{\beta_i\}_{i=1}^d$  are a collection of independent Wiener processes. Were they constant vectors, (14) could be couched in the form of a geodesic equation. Furthermore, upon converting (14a) to the Itô representation we

recover (13) for vanishing covariant drift. An important further consequence of (14a) is that we can identify a stochastic process  $\xi$  as a local  $\mathbb{M}$ -valued martingale if in any local chart it satisfies [19, 29, 37]

$$\begin{aligned} d\xi_t + \frac{1}{2}\Gamma : d\xi_t \otimes d\xi_t &\stackrel{law}{=} \\ d\xi_t + \frac{1}{2}\Gamma : g^{-1}dt &= \text{local Euclidean martingale} \end{aligned} \quad (15)$$

Three remarks are in order before concluding this short discussion of background results from stochastic analysis. First, (14) admits a straightforward extension to semi-martingales, simply by introducing a drift term into (14a). We do not need to take this step here explicitly, since we can combine Girsanov formula and the development map (14) to take into account drift terms [18]:

$$\begin{aligned} \frac{dP_\xi}{dP_\omega}(\omega) &= e^{\int_{t_o}^{t_f} \left\{ \langle \mathbf{b}, \mathbf{e}_{i;t} d\beta_{i;t} \rangle_g - \frac{\|\mathbf{b}\|_g^2}{2} dt \right\}}(\omega_t, t) \\ &= e^{\int_{t_o}^{t_f} \left\{ \langle d\mathbf{b} \circ \omega_t \rangle_g - \frac{(\nabla \cdot \mathbf{b} + \|\mathbf{b}\|_g^2)}{2} dt \right\}}(\omega_t, t) \end{aligned} \quad (16)$$

for

$$\nabla \cdot \mathbf{b} = \frac{1}{\sqrt{|g|}} \partial_{x^\alpha} (\sqrt{|g|} b^\alpha) \quad (17)$$

The symbol  $\nabla$  betokens here and in what follows the covariant derivative operation compatible with the metric  $g$ . The stochastic integral in the first row of (16) is in Itô sense. The use of the time-symmetric Stratonovich integral in the second row of (16) exhibits that the argument of the exponential transforms indeed as a scalar under a change of coordinates. Second, if the metric is time dependent we must include a drift term  $1/2 \partial_t g^{-1}$  in (14b) to preserve the metric compatibility of the connection. Finally [22] the adjoint of (8)

$$\mathcal{L}^\dagger f = -\nabla \cdot \mathbf{b}f + \frac{1}{2} \Delta_{LB} f \quad (18)$$

is defined with respect to the invariant Riemann volume:

$$d_{\mathbb{M}}x := d^d x \sqrt{\det g}(x) \quad (19)$$

The covariant density  $k$  is then related to the transition probability density with respect to the Lebesgue measure  $p$  by the equation

$$p(\mathbf{x}_2, t_2 | \mathbf{x}_1, t_1) = \sqrt{\det g}(\mathbf{x}_2) k(\mathbf{x}_2, t_2 | \mathbf{x}_1, t_1) \quad (20)$$

for any coordinates  $\mathbf{x}_i$ ,  $i = 1, 2$  in a local chart  $\mathbb{U}$ , and any  $t_2 \geq t_1$  in  $[t_o, t_f]$ .

## KULLBACK-LEIBLER DIVERGENCE AND TIME-REVERSAL

Our aim is now to derive with the help of the development map the covariant expression of time reversal relations which can be used as bridge relations between the theory of stochastic processes and finite-time

thermodynamics of small systems. Under rather general smoothness assumptions [35, 36], if we know the probability  $m = \sqrt{|g|}n$  and transition probability densities  $p = \sqrt{|g|}k$  of a semi-martingale process  $\xi$  in the full time horizon  $[t_f, t_o]$ , we can construct the time reversed time evolution by requiring for any  $t_o \leq t_1 \leq t_2 \leq t_f$

$$n(\mathbf{x}_2, t_2) k^{(r)}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) = k(\mathbf{x}_2, t_2 | \mathbf{x}_1, t_1) n(\mathbf{x}_1, t_1) \quad (21)$$

If  $\xi$  is adapted to a  $\mathbb{M}$ -valued Wiener process (14), we can use Girsanov formula (16) to evaluate averages of non-anticipative functionals of  $\xi$  as averages with respect to  $\omega$ . As noticed in [30], we can also take advantage of the invariance under time reversal of the Wiener process to express the density of a *backward* process  $\tilde{\xi} = \{\tilde{\xi}_t; t \in [t_o, t_f]\}$ :

$$\begin{aligned} \frac{dP_{\tilde{\xi}}}{dP_\omega}(\omega) &= e^{\int_{t_o}^{t_f} \left\{ \langle \tilde{\mathbf{b}}, \mathbf{e}_{i;t} \triangleright d\beta_{i;t} \rangle_g - \frac{\|\tilde{\mathbf{b}}\|_g^2}{2} dt \right\}}(\omega_t, t) \\ &= e^{\int_{t_o}^{t_f} \left\{ \langle d\tilde{\mathbf{b}} \circ \omega_t \rangle_g + \frac{(\nabla \cdot \tilde{\mathbf{b}} - \|\tilde{\mathbf{b}}\|_g^2)}{2} dt \right\}}(\omega_t, t) \end{aligned} \quad (22)$$

The symbol  $\triangleright$  appearing in the first row of (22) indicates that the stochastic integral is defined by taking the limit of Riemann sums sampled according to the post-point discretization; in other words, the first stochastic integral in (22) is an Itô integral with respect to the filtration of the “future” while the second is a Stratonovich integral.

The requirement  $\xi \stackrel{law}{=} \tilde{\xi}$  translates into

$$n(\omega_{t_2}, t_2) \frac{dP_{\tilde{\xi}}}{dP_\omega}(\omega) = n(\omega_{t_1}, t_1) \frac{dP_\xi}{dP_\omega}(\omega) \quad (23)$$

whence we immediately recover the classical result

$$\mathbf{b}(\mathbf{x}, t) = \tilde{\mathbf{b}}(\mathbf{x}, t) + g^{-1} \cdot \partial_x n(\mathbf{x}, t) \quad (24)$$

Both sides of the equation are now well-defined vector fields. We thus see that the *same* probability measure admits a forward and backward dynamics representation in terms of two *different* drift vector fields. A natural way to compare the two vector fields with respect to the same filtration is to introduce a *forward, auxiliary* process  $\bar{\xi}$  *absolutely continuous* with respect to  $\xi$  defined by the replacement

$$\mathbf{b} \mapsto \bar{\mathbf{b}} := -\tilde{\mathbf{b}} \quad (25)$$

in the stochastic differential equation driving  $\xi$ . The rationale behind (25) is to combine the stochastic with deterministic time reversal. As a consequence, for a gradient-type drift (see equation (33) below) at equilibrium (25) reduces to the identity  $\mathbf{b} = \bar{\mathbf{b}}$ . In general a natural quantifier of the “drift discrepancy” is obtained by considering the Kullback-Leibler divergence [23] of the process  $\bar{\xi}$  with respect to  $\xi$ :

$$\begin{aligned} \mathcal{K}(P_{\bar{\xi}} || P_\xi) &:= E^{(\xi)} \ln \frac{dP_{\bar{\xi}}}{dP_\xi}(\xi) \\ &= E^{(\omega)} \frac{dP_\xi}{dP_\omega}(\omega) \ln \left( \frac{dP_{\bar{\xi}}}{dP_\omega} \frac{dP_\omega}{dP_\xi} \right)(\omega) \end{aligned} \quad (26)$$

The notation  $E^{(\xi)}$  ( $E^{(\omega)}$ ) emphasizes that the average is with respect to the measure of  $\xi$  ( $\omega$ ). The Kullback-Leibler divergence is by construction a positive definite quantity. Direct evaluation of (26) yields

$$\begin{aligned} \mathcal{K}(P_{\tilde{\xi}}||P_{\xi}) &= E^{(\xi)} \int_{t_o}^{t_f} \langle \mathbf{b} + \tilde{\mathbf{b}} \diamond d\xi_t \rangle_{\mathbf{g}} \\ &- E^{(\xi)} \int_{t_o}^{t_f} dt \frac{\nabla_{\xi_t} \cdot (\mathbf{b} + \tilde{\mathbf{b}}) + \|\mathbf{b}\|_{\mathbf{g}}^2 - \|\tilde{\mathbf{b}}\|_{\mathbf{g}}^2}{2} \end{aligned} \quad (27)$$

Upon inserting (24) into (27) and using probability conservation and the covariant Fokker-Planck equation

$$(\partial_t - \mathfrak{L}^\dagger)\mathbf{n} = 0 \quad (28)$$

we can prove that the Riemann integral in (27) vanishes. The integrand of the Stratonovich stochastic integral is instead proportional to the *current velocity* [35, 36] of the process  $\xi$ :

$$\mathbf{v} = \frac{\mathbf{b} + \tilde{\mathbf{b}}}{2} \quad (29)$$

The current velocity enjoys two important properties. First, it plays for expectation values of Stratonovich line integrals the same role as the Itô drift (5) for expectation values of Itô line integrals: for any smooth, mean square integrable vector field  $\mathbf{h}$  the equality

$$E^{(\xi)} \int_{t_o}^{t_f} \langle \mathbf{h} \diamond d\xi \rangle_{\mathbf{g}} = E^{(\xi)} \int_{t_o}^{t_f} dt \langle \mathbf{h}, \mathbf{v} \rangle_{\mathbf{g}} \quad (30)$$

holds true under the assumption that integrations by parts do not bring about boundary terms. Second, in terms of the current velocity the covariant Fokker-Planck equation reduces to deterministic mass conservation equation:

$$\partial_t \mathbf{n} + \nabla \cdot \mathbf{v} \mathbf{n} = 0 \quad (31)$$

Combining (30) with (24) and (28) we finally arrive at

$$\mathcal{K}(P_{\tilde{\xi}}||P_{\xi}) = 2 E^{(\xi)} \int_{t_o}^{t_f} dt \|\mathbf{v}\|_{\mathbf{g}}^2 \quad (32)$$

The right hand side of (32) is proportional to the “kinetic energy” specified by the current velocity of the system. Its physical interpretation [2, 27] (see also [7, 13, 41]) is that of *entropy production* during the transformation. The way we arrived to (32) differs to some extent from the one of [24, 26, 28]. There the role of the Kullback-Leibler divergence is played by an “action functional” defined by contrasting the forward dynamics with its path-space time reversed defined by inverting the arrow of time  $t \mapsto t_f + t_o - t$  in analogy to what was done to prove fluctuation theorems in hyperbolic dynamics [12]. The entropy production relation can also be regarded as the continuum limit under diffusive scaling of the analogous relation found in [34] for Markov jump processes.

## STOCHASTIC THERMODYNAMICS

Let us now examine the consequences of (32) for optimal control in thermodynamic functionals. We thus consider a dynamical system driven by time-dependent gradient-like drift

$$\mathbf{b}(\mathbf{x}, t) = -\mathbf{g}^{-1}(\mathbf{x}) \cdot \partial_{\mathbf{x}} U(\mathbf{x}, t) \quad (33)$$

which is a stylized model of a mechanical potential subject to an external control. The current velocity becomes in such a case

$$\mathbf{v}(\mathbf{x}, t) = -\mathbf{g}^{-1}(\mathbf{x}) \cdot \partial_{\mathbf{x}} \left( U + \frac{1}{2} \ln \mathbf{n} \right) (\mathbf{x}, t) \quad (34)$$

Drawing from [42], we define the work done on the system as

$$\begin{aligned} \mathcal{W}_{t_f, t_o} &= E^{(\xi)} \int_{t_o}^{t_f} dt \partial_t U(\xi_t, t) = E^{(\xi)} U(\xi_t, t)|_{t_o}^{t_f} \\ &- E^{(\xi)} \int_{t_o}^{t_f} \langle d\xi_t \diamond \mathbf{g}^{-1}(\xi_t) \cdot \partial_{\xi_t} U(\xi_t, t) \rangle_{\mathbf{g}} \end{aligned} \quad (35)$$

If we require the first law of thermodynamics to hold true, we must identify the heat as

$$\mathcal{Q}_{t_f, t_o} = -E^{(\xi)} \int_{t_o}^{t_f} \langle d\xi_t \diamond \mathbf{g}^{-1}(\xi_t) \cdot \partial_{\xi_t} U(\xi_t, t) \rangle_{\mathbf{g}} \quad (36)$$

Under the present conventions, the local equilibrium condition is

$$\nabla_{\mathbf{x}} \cdot \mathbf{g}^{-1} \cdot \left( \mathbf{n} \partial_{\mathbf{x}} U + \frac{1}{2} \partial_{\mathbf{x}} \mathbf{n} \right) = 0 \quad (37)$$

Correspondingly, we define the osmotic velocity [35, 36] as

$$\begin{aligned} \mathbf{u}(\mathbf{x}, t) &:= \frac{1}{2} (\mathbf{b} - \tilde{\mathbf{b}})(\mathbf{x}, t) \\ &= \frac{1}{2} \mathbf{g}^{-1}(\mathbf{x}) \cdot \partial_{\mathbf{x}} \ln \mathbf{n}(\mathbf{x}, t) \end{aligned} \quad (38)$$

and the scalar (i.e. coordinate independent) expression of the Gibbs-Shannon entropy

$$\begin{aligned} \mathcal{S}(t) &= -\frac{1}{2} E^{(\xi)} \ln \mathbf{n}(\xi_t, t) \\ &\equiv -\frac{1}{2} \int_{\mathbb{M}} d_{\mathbb{M}}^d x (\mathbf{n} \ln \mathbf{n})(\mathbf{x}, t) \end{aligned} \quad (39)$$

Note that the definition (39) of the Gibbs-Shannon entropy differs from the one given in [2, 4] by a prefactor 1/2 dictated by the convention adopted here for the diffusion tensor, and by an addend proportional to  $\ln \sqrt{|\mathbf{g}|}$  which does not transform as a scalar under change of coordinates. If we now add and subtract the osmotic velocity to the integrand in (35) and (36), use probability conservation and the identity (30), we arrive at the

manifestly coordinate-independent representations of the released heat

$$\mathcal{Q}_{t_f, t_o} = -[\mathcal{S}(t_f) - \mathcal{S}(t_o)] + E^{(\boldsymbol{\xi})} \int_{t_o}^{t_f} dt \|\mathbf{v}\|_{\mathbf{g}}^2 \quad (40)$$

and of thermodynamic work

$$\mathcal{W}_{t_f, t_o} = \mathcal{F}(t_f) - \mathcal{F}(t_o) + E^{(\boldsymbol{\xi})} \int_{t_o}^{t_f} dt \|\mathbf{v}\|_{\mathbf{g}}^2 \quad (41)$$

In (41) the Helmholtz free energy of the system is

$$\mathcal{F}(t) \equiv \mathcal{U}(t) - \mathcal{S}(t) = E^{(\boldsymbol{\xi})} \left( U + \frac{1}{2} \ln n \right) (\boldsymbol{\xi}_t, t) := -E^{(\boldsymbol{\xi})} \psi(\boldsymbol{\xi}_t, t) \quad (42)$$

The advantage to introduce here the *scalar* quantity  $\psi$  to denote the free energy density emerges when contrasting the definitions of the current and osmotic velocities with (33). We recognize then that the current velocity is the gradient of the Helmholtz free energy density:

$$\mathbf{v}(\mathbf{x}, t) = \mathbf{g}^{-1}(\mathbf{x}) \cdot \partial_{\mathbf{x}} \psi(\mathbf{x}, t) \quad (43)$$

It is worth noticing that the Helmholtz free energy  $\psi$  density (42) coincides with the potential similarly denoted in [4] owing to a cancellation of terms proportional to  $\ln \sqrt{|\mathbf{g}|}$  between the individually non-coordinate-independent expressions of the internal energy and the Gibbs-Shannon entropy thereby used. Similar considerations, exploiting the time-independence of the Riemann metric also guarantee that the expression for the released heat of [4] does coincide with the one given here. The same is true for the work whose expression (41) has been obtained also in [6] using, however, arguments valid only in the weak noise limit.

## OPTIMAL CONTROL

The expressions (40) and (41) evince that the current velocity formulation of Langevin thermodynamics is natural from the point of view of control theory. There are at least two kinds of considerations supporting this claim. First, by (31) the current velocity maps the original stochastic control problem into a deterministic control one. Such a mapping exists for any smooth diffusion but it is of limited practical use if the drift is known a-priori and the problem is to derive the evolution of the density. It becomes useful for control purposes when the drift is not known but must be determined by minimizing a “cost” functional over a suitable space of admissible controls. The second consideration is that the functional dependence of the entropy production on the current velocity readily enforces the *coercivity condition* (see e.g. [11] pag. 33: convexity with growth faster than linear) which plays an important role in variational calculus to

prove the existence of extremal solutions. A direct consequence of these considerations is the recovery of Jarzynski’s

$$\mathcal{W}_{t_f, t_o} \geq \mathcal{F}(t_f) - \mathcal{F}(t_o) \quad (44)$$

and “finite-time Landauer’s” [25] inequalities

$$\mathcal{Q}_{t_f, t_o} \geq -[\mathcal{S}(t_f) - \mathcal{S}(t_o)] \quad (45)$$

The interpretation of (45) as Landauer’s inequality stems from the identification of the heat release with the entropy variation of the environment. By (34) the current velocity vanishes at equilibrium. As a consequence, the inequalities (44), (45) become tight for transitions described by a *jump* between two “equilibrium” states. Physically, jumps are mathematical mock-up’s for transitions occurring at the fastest admissible time-scale. As such, they are not suited to describe macroscopic control of a nano-system. It is therefore relevant to look for minima of thermodynamics indicators by restricting the space of admissible controls to those guaranteeing a smooth behavior of the current velocity. In order to achieve this goal let us recall that given a forward Markov process  $\boldsymbol{\eta}$ , deterministic or stochastic, with generator  $\mathfrak{G}_{[\mathbf{u}]}$  depending on a control  $\mathbf{u}$ , the canonical form of cost functionals considered in control theory [11] is

$$\mathcal{A}(\mathbf{x}, t) = E_{\mathbf{x}, t}^{(\boldsymbol{\eta})} \Psi(\boldsymbol{\eta}_{t_f}) + E_{\mathbf{x}, t}^{(\boldsymbol{\eta})} \int_t^{t_f} dt L(\boldsymbol{\eta}_t, t; \mathbf{u}) \quad (46)$$

Standing some regularity assumptions, it is a-priori tenable to expect the “cost functional”  $\mathcal{A}$  to admit a minimum over the space of smooth controls  $\mathbf{u}$  if the “running cost”  $L$  depends coercively on  $\mathbf{u}$  and the “terminal cost”  $\Psi$  is some assigned function independent of  $\mathbf{u}$ . The minimum

$$J_{\star}(\mathbf{x}, t) = \min_{\mathbf{u}} \mathcal{A}(\mathbf{x}, t) \quad (47)$$

is usually referred to as the “value function”. Under these hypotheses, the solution of the Hamilton-Jacobi-Bellman equation

$$\partial_t J_{\star} + \min_{\mathbf{u}} \{ \mathfrak{G}_{[\mathbf{u}]} J_{\star} + L \} = 0 \quad (48a)$$

$$J_{\star}(\mathbf{x}, t_f) = \Psi(\mathbf{x}) \quad (48b)$$

corresponding to the smallest value of  $\mathcal{A}$  (in case of multiple minima in (48a)) specifies the value of the optimal control  $\mathbf{u}_{\star}$  for any  $t$  in a *closed* horizon  $[t_o, t_f]$  if the resulting  $\mathfrak{G}_{[\mathbf{u}_{\star}]}$  is a well-defined generator of a Markov process. The properties that a solution of (48) must enjoy in order to satisfy such self-consistency condition are determined by so called *verification theorems* [11, 45]. Linearity of the Kolmogorov pair of equations governing a Markovian dynamics extends (48) to expectations

of  $\mathcal{A}$  with respect to the measure of  $\boldsymbol{\eta}$  evolving from non-localized initial density assigned at time  $t = t_o$  [15]. Namely, if we denote variations with respect to the control  $\mathbf{u}$  by a “prime symbol”, we can couch the variation of  $E^{(\boldsymbol{\eta})}\mathcal{A}$  into the form

$$(E^{(\boldsymbol{\eta})}\mathcal{A})'(\boldsymbol{\eta}_{t_o}, t_o) = \int_{\mathbb{M}} d_{\mathbb{M}}^d x (n'_{\boldsymbol{\eta}} \Psi)(\mathbf{x}, t) + \int_{t_o}^{t_f} dt \int_{\mathbb{M}} d_{\mathbb{M}}^d x (n'_{\boldsymbol{\eta}} L + n_{\boldsymbol{\eta}} L')(\mathbf{x}, t) \quad (49)$$

If we now require the “dynamic programming” (non-homogeneous backward Kolmogorov) equation to hold for any admissible control

$$(\partial_t + \mathfrak{G}_{[\mathbf{u}]})J + L = 0 \quad (50)$$

we obtain for  $n'_{\boldsymbol{\eta}}(\cdot, t_o) = 0$

$$(E^{(\boldsymbol{\eta})}\mathcal{A})' = \int_{\mathbb{M}} d_{\mathbb{M}}^d x [n'_{\boldsymbol{\eta}} (\Psi - J)](\mathbf{x}, t) + \int_{t_o}^{t_f} dt \int_{\mathbb{M}} d_{\mathbb{M}}^d x \left\{ J [(\partial_t - \mathfrak{G}_{[\mathbf{u}]})n_{\boldsymbol{\eta}}]' \right\}(\mathbf{x}, t) + \int_{t_o}^{t_f} dt \int_{\mathbb{M}} d_{\mathbb{M}}^d x \left\{ n_{\boldsymbol{\eta}} (\mathfrak{G}'_{[\mathbf{u}]} J + L') \right\}(\mathbf{x}, t) \quad (51)$$

The variation yields a stationary point if (48b) is satisfied, the probability density evolves for any  $\mathbf{u}$  according to the dynamics specified by the adjoint action of  $\mathfrak{G}_{[\mathbf{u}]}$ , and the optimal control is fixed by the same condition as in (48a). If, furthermore, the generator is linear in the control  $\mathbf{u}$ , the convexity of  $L$  readily implies that the stationary point is a minimum

$$(E^{(\boldsymbol{\eta})}\mathcal{A})'' = \int_{t_o}^{t_f} dt \int_{\mathbb{M}} d_{\mathbb{M}}^d x (n_{\boldsymbol{\eta}} L'')(\mathbf{x}, t) \geq 0 \quad (52)$$

The dynamic programming equation (50) has the hydrodynamic interpretation of a material derivative along the realizations of the Markov process  $\boldsymbol{\eta}$ . Requiring it to hold a priori substantiate Bellman’s idea that optimal control stems from a condition imposed *locally* during the time evolution [11, 45]. Within this framework, probability evolution must be regarded as the adjoint transport equation which may-be non-local owing to the boundary conditions and must hold in the same time horizon  $[t_o, t_f]$  where (50) is defined. In [15] it was also shown that the above chain of steps holds also if the running cost  $L$  depends upon derivatives of the control. This fact was originally exploited in [3] to unveil the relation between optimal thermodynamic control and hydrodynamic mass transport. The formulation in terms of the current velocity renders, however, this extension no further needed for thermodynamic control.

In the application of the control-theory toolkit to expressions such as (41) we are confronted with a subtle

difficulty. While the entropy production specifies a well-defined coercive running cost, the interpretation of the terminal cost is more problematic. Namely, a candidate smooth optimal control must satisfy the stationarity condition

$$\partial_{\mathbf{x}} J_{\star} + 2 \mathbf{g} \cdot \mathbf{v} = \partial_{\mathbf{x}} (J_{\star} + 2 \psi) = 0 \quad (53)$$

and the terminal condition (we suppose that no optimization is carried out over the initial state)

$$J_{\star}(\mathbf{x}, t_f) = \Psi(\mathbf{x}) \quad (54)$$

Contrasting (53) and (54) with (43) it is evident that the terminal condition *cannot* be interpreted as the end-horizon value of the free energy density of a *smooth optimal* protocol since in general  $\psi(\cdot, t_f) \neq \Psi(\cdot)$ . Furthermore, a process jumping at  $t_f^-$  from a state of *non-vanishing* current velocity *cannot* be considered *optimal*, independently of the prescription adopted for the probability density at time  $t_f$ . Namely, if we enlarge the space of admissible protocols to encompass jump processes, we know a-priori that the infimum is attained by an instantaneous transition between “equilibria”. In this latter case the current velocity and the running cost vanish identically in the full control horizon and the work coincides with the free energy difference. The conclusion is that the “optimal work” protocol proposed in [39] *cannot* be justified using Hamilton-Jacobi-Bellman theory and Langevin dynamics alone. It appears instead to describe an optimal control strategy if the Langevin dynamics is embedded into an higher order Markovian dynamics [4] following ideas closely reminiscent of the “valley method” (see e.g. [1]). The “valley method” is a technique which aims at justifying the stationary point approximation to path integrals when no exact classical field configuration can match the required boundary conditions. It is worth stating clearly that if the terminal cost (54) is interpreted only as the variation of an external potential without explicit relation with  $\psi$  in the control horizon  $[t_o, t_f]$  then the protocol found in [4, 39] is optimal according to standard verification theorems (see e.g. discussion in sections III.5 to III.8 of [11]).

A control problem which lends itself to a more transparent physical interpretation is that of the minimization of the entropy production between assigned probability densities at the end of the control horizon. The analytical and numerical treatment of this problem have been inquired in details in [2]. It is worth here to draw the attention some aspects of this problem not discussed in [2, 4]. By (32) the problem can be equivalently formulated in terms of the minimization of the Kullback-Leibler divergence associated to a time reversal operation. It is instructive to contrast thermodynamic entropy production minimization with the control problem defining the so-called “Schrödinger diffusion” see e.g. [9, 10, 31, 40]. Given two probability densities at the

end of a control horizon and a reference diffusion process, the Schrödinger diffusion problem determines the smoothly interpolating diffusion obtained from the reference process by a deformation of the drift under the requirement that the Kullback-Leibler divergence between the two processes be at a minimum value. If the reference process is the Wiener process then the Schrödinger diffusion corresponds to treat as running cost instead of the entropy production an analogous quantity in which the current velocity is replaced by the forward drift of the process. Correspondingly, the associated control problem is turned from deterministic to stochastic. A widely used approach to deterministic control is to prove existence and uniqueness of solutions in viscosity sense [11]. In simplest cases this means constructing solutions as the inviscid limit of an ultraviolet regularization of the Hamilton-Jacobi equation by adding a Laplacian. The Monge-Ampère-Kantorovich method [32] applied in [2] to study nucleation at minimum entropy production is an example of this general ideology. This observation allows us to attribute a direct physical interpretation also to the regularized entropy production minimization problem. Namely, in the presence of any finite viscosity we can interpret the minimizer of the Kullback-Leibler divergence (32) as the drift solving an associated Schrödinger diffusion problem.

## CONCLUSIONS

In conclusion, we showed how a coordinate independent formalism for stochastic differential equations provides a convenient formulation of control problems arising in stochastic thermodynamics. In doing so we restricted the attention to time-independent diffusion tensors. This is not too restrictive under the hypothesis that mechanical forces and control parameters are most naturally encapsulated in the drift field whilst the diffusion coefficient contains purely geometric information. We also analyzed how the local nature of Bellman principle affects the optimal control equations. Preserving the adjoint structure of the Kolmogorov pair requires for example that jumps in the protocol which is governed by the backward Kolmogorov equation bring about jumps in the forward Kolmogorov equation governing the probability density evolution. Hence, it is an essential modeling question to assess a-priori which is the physically relevant space of admissible protocols and whether and how to describe the procedures to switch on and off the optimal protocol at the end of the control horizon.

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